Laplacian-Based Models for the Exchange Energy

A. C. Cancio[1] and C. E. Wagner[1,2]

[1] *Department of Physics and Astronomy, Ball State University, Muncie, IN 47306, USA.*
[2] *Currently at Department of Physics, University of Florida, FL, USA.*

Recent Quantum Monte Carlo data for the exchange-correlation energy density of pseudopotential systems strongly indicate the significant role of the Laplacian of the density in characterizing the first order correction to the local density approximation of density functional theory. We report on an exchange functional built upon these observations and extended to the all-electron case. The model keeps the typical properties of constraint-based generalized gradient approximations (GGA) and also has a finite-valued potential at the nucleus, unlike the GGA. Problems with oscillatory behavior in the potential due to higher order derivatives are controlled by a curvature minimization constraint. The results are tested against exact potentials for the He, Be, and Ne atoms. A combination of gradient and Laplacian as suggested by a gradient expansion of the exchange hole gives the best overall results.

This work is funded by NSF grant DMR-0812195.

Contact: accancio@bsu.edu